

Extensions of the TEP Neutral Transport Methodology

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Abstract

Recent extensions of the Transmission and Escape Probability methodology and its implementation in the 2-D neutral transport code GTNEUT are presented. These extensions address the issues of anisotropy of the neutral distribution function at the interfaces and the non-uniformity of the first collision source in short mean free path regions. Comparisons with Monte Carlo for a number of model problems are discussed.

1. Introduction

The Transmission and Escape Probability (TEP) interface current balance method¹ has been developed and implemented into the 2-D neutral transport code GTNEUT to provide a fast and accurate calculation of neutral particle transport in the complex tokamak edge and divertor configuration.

Tests of GTNEUT predictions against Monte Carlo calculations and experimental measurements in DIII-D have demonstrated²⁻⁵ the accuracy and computational efficiency of the TEP method for a wide range of conditions. However, calculations of detailed model problems^{3,4} designed to test approximations in limiting cases have identified two main areas in which extensions in the original TEP methodology would be useful: 1) taking anisotropy into account in the calculation of first-flight transmission coefficients when the neutral mean free path (mfp) is much larger than the characteristic dimension of the computational region; and 2) taking into account that the escape of scattered or charge-exchanged neutrals is preferential across the incident surface when the mfp is small compared to the characteristic dimension of the computational region.

In this paper, we discuss recent extensions of the TEP methodology which address the above issues. The anisotropy of the neutral distribution function at the interfaces is taken into account by implementing Double P1 (DP₁) and Double P2 (DP₂) approximations. The preferential backscattering of scattered or charge-exchange neutrals across the incident surface is addressed by implementing an albedo-based condition to describe the fraction of the collided neutrals that are reflected back across the incident surface.

2. Extensions of the TEP methodology

Development of the DP₁ and DP₂ approximations

The original TEP methodology was based on the Double P0 (DP₀) approximation. This approximation assumes isotropic angular fluxes in both the inward and outward half-spaces at the interfaces between the computational regions for the purpose of calculating the first-flight transmission probabilities. Extensive comparisons with Monte Carlo indicate that DP₀ is a reasonable approximation when the neutral mean-free-path λ to grid size Δ ratio λ/Δ is small, since charge exchange and scattering collisions tend to isotropize the neutral distribution function. On the other hand, departure from isotropy is expected in long mean free path regions where anisotropies driven by wall reflection, presence of vacuum regions, pumps, etc. would persist across regions.

To improve the accuracy of the TEP method in cases where the neutral distribution function at the interfaces is expected to be anisotropic, the original DP₀ approximation was extended to include linearly (DP₁) and quadratically (DP₂) anisotropic distributions. Such cases have been extensively studied in neutron transport⁶⁻⁸ to model strongly heterogeneous fuel assemblies, such as those found in light water reactors.

Assuming that the neutral angular flux $\psi_{i,j}(\mathbf{r}_s, \mathbf{\Omega})$ at the interface \mathbf{r}_s between region i and region j can be expanded in a set of orthonormal angular representation functions $\psi_{i,j}^n$, we can write:

$$\psi_{i,j}(\mathbf{r}_s, \mathbf{\Omega}) = \sum_{n=0}^N \Gamma_{i,j}^n \psi_{i,j}^n(\mathbf{r}_s, \mathbf{\Omega}) \quad (1)$$

where $\Gamma_{i,j}^n$ is the n -th coefficient of the expansion⁷.

The coefficients of the angular expansion are the unknowns of the extended TEP theory and they satisfy a generalized set of interface balance equations:

$$\Gamma_{i,j}^n = \sum_{n'=0}^N \sum_k T_{i,k \rightarrow j}^{n' \rightarrow n} \Gamma_{k,i}^{n'} + \left(\sum_k \Gamma_{k,i}^0 - \sum_{n'=0}^N \sum_k \sum_l T_{i,k \rightarrow l}^{n' \rightarrow 0} \Gamma_{k,i}^{n'} \right) c_i P_i \Lambda_{ij} \delta_{n0} + S_i P_i \Lambda_{ij} \delta_{n0} \quad (2)$$

As in the original TEP formulation¹, the first term in Eq. (2) represents the uncollided part of the partial current, generalized to include contributions from all the other angular terms. The second term represents the collided contribution from neutrals that suffered one or more charge exchange or scattering collisions in region i and subsequently emerged into region j . It has been implicitly assumed that the collided contribution is isotropic. Finally, the third term represents any contributions from volumetric sources which are also assumed to be isotropic. The various coefficients appearing in Eq. 2, such as the total escape probability P_i , the charge exchange fraction c_i and the directionality factor Λ_{ij} , have the same meaning they had in the original theory¹⁻⁵.

The first flight transmission probability $T_{i,k \rightarrow j}^{n' \rightarrow n}$ in 2D geometry is calculated from:

$$T_{i,k \rightarrow j}^{n' \rightarrow n} = \pi S_j \int_{\partial D_j} dS \int_{\partial D_k} dS' \psi_{i,j}^n(\mathbf{r}_s, \mathbf{\Omega}_j) \psi_{k,i}^{n'}(\mathbf{r}'_s, \mathbf{\Omega}_k) \frac{\exp[-\tau(\mathbf{r}_s, \mathbf{r}'_s)]}{R^2} (\mathbf{\Omega} \cdot \mathbf{n}_{ij})(\mathbf{\Omega} \cdot \mathbf{n}_{ki}) \quad (3)$$

Where S_j is the area of the interface between region i and region j , ∂D denotes the interface, and R is the distance between points \mathbf{r}_s and \mathbf{r}'_s .

Directional escape probability correction

The original TEP methodology assumes that the charge exchange collision source, which is responsible for the collided term in the partial current balance equations, is uniformly distributed within each region. This assumption is embodied in the rational approximation that we use for the first flight collision probability P_{0i} , and more importantly in the treatment of the geometry factors Λ_{ij} which lack any specific directionality, being instead proportional to the fractional perimeter of each interface. Detailed comparisons with Monte Carlo indicate that this is a good approximation, as long as the neutral mean free path is comparable to or larger than the characteristic dimension of each region. However, in short mean free path regions, the first collision source is predominantly located near the incident interface, resulting in a preferential backscattering of these neutrals across that incident surface, which is not represented in the original formulation.

A simple way to remedy this situation is to reduce the size of the computational regions, ensuring that λ/Δ is always ≥ 1 . However, being able to deal with $\lambda/\Delta < 1$ cases without loss of accuracy is very

desirable for flexibility and for being able to deal with changing background plasma conditions in dynamic simulations.

An exact treatment of this problem would require the direct calculation of the first collision escape probability assuming a non-uniform first collision source. However, this is impractical since the exact distribution of the first collision source is unknown and, even if it were known, the additional computation time required for the evaluation of the 3-D escape probability integrals would adversely affect the computational performance of the code. For these reasons, an approximate approach has been adopted based on the concept of the *albedo* coefficient.

If the neutral mfp is much smaller than the characteristic dimension of region i , we can treat it as an infinite half space and express the fraction of the collided particles that is scattered back across the incident surface k in terms of the albedo coefficient. Using an analytic expression for the albedo coefficient from neutron diffusion theory⁹, the modified directionality factor Λ_{ik} for the incident surface becomes:

$$\Lambda_{i,k}^k = \frac{1 - \frac{2}{\sqrt{3}} \sqrt{c_{i,k}^{-1} - 1}}{1 + \frac{2}{\sqrt{3}} \sqrt{c_{i,k}^{-1} - 1}} \frac{1}{c_i P_i \left(1 - \sum_l T_{k,l}^i \right)} \quad (4)$$

where the superscript k denotes the region of origin of the neutrals and $c_{i,k}$ is the charge exchange collision fraction of neutrals entering region i from region k . Directional escape from the other sides of region i is treated as before, i.e. it is proportional to the perimeter fraction of each interface:

$$\Lambda_{i,j}^k = \frac{l_{i,j} (1 - \Lambda_{i,k}^k)}{l_i - l_{i,k}} \quad (5)$$

In Eq. 6, $l_{i,j}$ is the length of the side of region i that is adjacent to region j , l_i is the perimeter of region i and the correction factors ensure that the preferential treatment of the k -th interface is taken into account.

It should be noted that the analytic expression for the albedo coefficient in Eq. (4) becomes negative for charge exchange fractions $c_{i,k}$ less than 0.57. This limitation is due to the diffusion theory origin of Eq. (4). We are in the process of developing a transport theory estimate of the albedo coefficient.

3. Comparison with Monte Carlo

To test the accuracy of the DP₁ and DP₂ approximations, comparisons with the Monte Carlo neutral transport code DEGAS¹⁰ have been carried out for a number of model problems with simplified geometries. In order to accentuate the anisotropy effects and avoid any other potential causes of discrepancy such as those associated with the calculation of escape probabilities, we have considered neutral transport in a purely ionizing medium, i.e. charge exchange and elastic scattering, which would isotropize the distribution, are neglected. Similarly, to exclude effects introduced by wall reflection, only vacuum boundary conditions are employed.

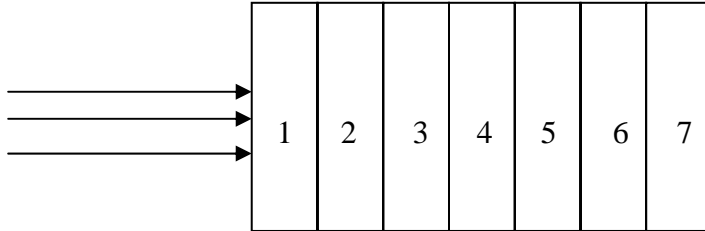


Figure 1: 1-dimensional slab geometry (2.1 m length \times 0.9 m height) with $\lambda/\Delta = 0.5$.

Two different geometric configurations have been considered. The first, shown in Fig. 1, consists of a 1-dimensional slab geometry configuration with a uniform source of neutrals of unit strength ($1 \text{ \#/m}^2\text{-s}$) at the left boundary, and a uniform background plasma with properties adjusted so that the ratio λ/Δ is equal to 0.5. The results of the simulation for this case are shown in Fig. 2, where the neutral density for each region is plotted. The four different curves in Fig. 2 correspond to Monte Carlo (DEGAS), the original GTNEUT code (DP_0) and the GTNEUT code with the DP_1 and DP_2 approximations. It can be seen that the GTNEUT simulations with the DP_1 and DP_2 approximations agree very well with Monte Carlo throughout the entire region, while the original GTNEUT with the DP_0 approximation diverges from the Monte Carlo solution after about 4-6 mean free paths away from the source. This is due to the fact that as we move away from the source in a purely ionizing medium, a forward peaking of the neutral distribution function at the interfaces is expected due to the enhanced attenuation of neutrals with long flight paths, corresponding to large angles relative to the normal. Similar results have been obtained for other cases with different λ/Δ ratios and with finite charge exchange fractions, although the isotropizing effect of charge exchange collisions helps to significantly reduce the differences between the original DP_0 methodology and the DP_1 and DP_2 extensions.

To extend our comparison with Monte Carlo to problems with strong 2-D effects, a $0.9 \text{ m} \times 0.9 \text{ m}$ rectangular region with nine cells has been considered (Fig. 3). As in the previous case, a pure absorbing medium is assumed and the λ/Δ ratio is taken to be equal to 1. Vacuum boundary conditions are assumed and a surface source of unit strength is imposed at the left boundary of region 2. The results of this simulation are shown in Fig. 4. As in the previous case, it can be seen that the DP_1 and DP_2 approximations agree very well with Monte Carlo throughout the entire region of interest, while the DP_0 approximation deviates from the correct solution in regions away from the source.

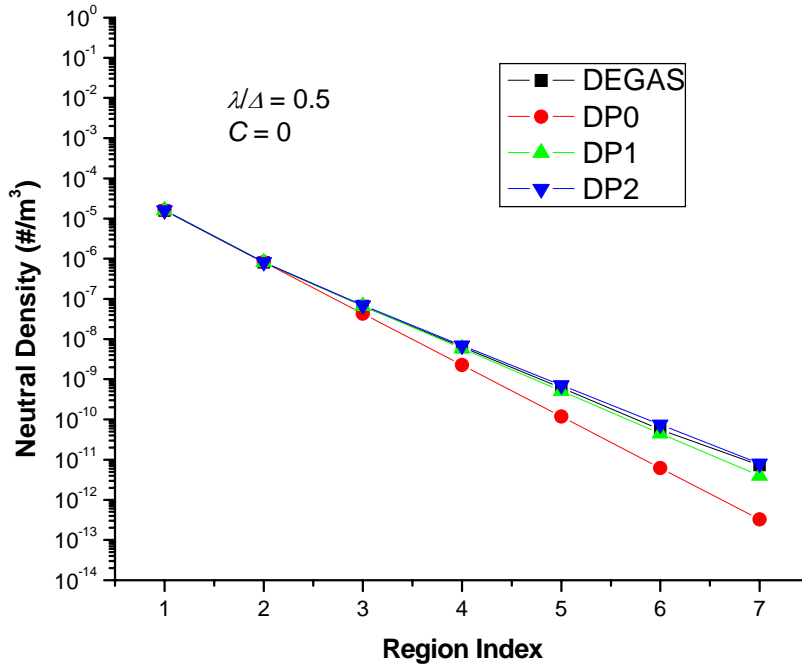


Figure 2: Neutral densities vs. region index for the geometry of Fig. 1 and for the case with $\lambda/\Delta = 0.5$ and including only ionization (charge exchange collision fraction, $c = 0$).

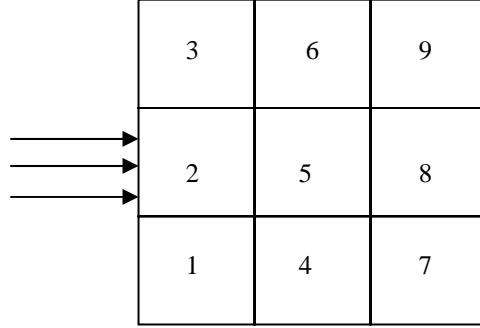


Figure 3: Geometry for the 2-D nine region configuration with $\lambda/\Delta = 1.0$

To test the accuracy of the directional escape probability correction, a problem similar to that described by the geometry of Fig. 3 but with a charge exchange collision fraction $c = 0.9$ is analyzed with the Monte Carlo code DEGAS, the original GTNEUT code (DP₀ approximation), the GTNEUT code with the DP₁ approximation and the GTNEUT code with the DP₁ and albedo approximations. The results of these simulations are shown in Fig. 5. It can be seen that 1) the original DP₀ approximation is adequate and not improved by the DP₁ approximation, and 2) the albedo correction improves agreement between the TEP method and Monte Carlo in regions away from the source.

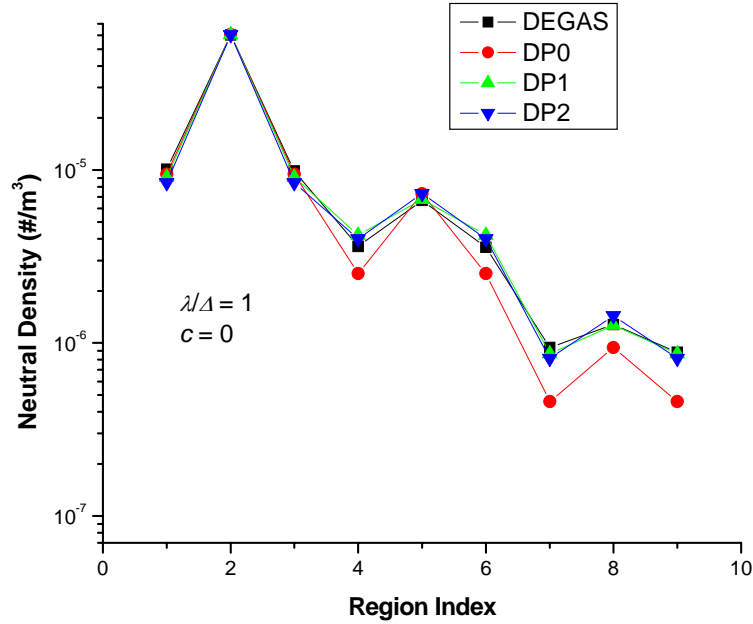


Figure 4: Neutral densities vs. region index for the 3×3 region problem of Fig. 3.

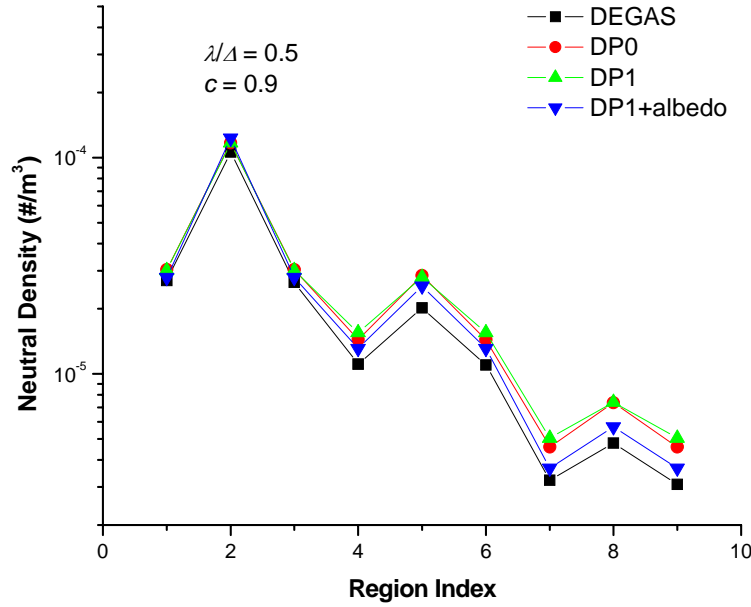


Figure 5: Neutral densities vs. region index for various assumptions

4. Conclusions

The Transmission and Escape Probabilities (TEP) methodology has been extended to include 1) the effects of angular anisotropy of the neutral distribution function at the interfaces via the implementation of DP₁ and DP₂ approximations and 2) the effect of a non-uniform first collision source via the use of albedo coefficients. Benchmarking calculations with Monte Carlo indicate that the DP₁ calculation is significantly better than the original DP₀ calculation for model problems chosen to accentuate anisotropy, but there is little advantage to further extending the calculation to DP₂. Preliminary comparisons with Monte Carlo for problems with short mean free paths compared to the size of the computational region indicate improved accuracy when the albedo correction is included in the calculation of the directional escape probabilities.

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